



# UNITED STATES PATENT AND TRADEMARK OFFICE

UNITED STATES DEPARTMENT OF COMMERCE  
United States Patent and Trademark Office  
Address: COMMISSIONER FOR PATENTS  
P.O. Box 1450  
Alexandria, Virginia 22313-1450  
www.uspto.gov

APPLICATION NO.	FILING DATE	FIRST NAMED INVENTOR	ATTORNEY DOCKET NO.	CONFIRMATION NO.
09/506,717	02/18/2000	Harold E Helson	103544.127	9161

7590

10/23/2003

Jason A Reyes  
Hale and Dorr LLP  
60 State street  
Boston, MA 02109

EXAMINER

MARSCHER, ARDIN H

ART UNIT

PAPER NUMBER

1631

DATE MAILED: 10/23/2003

Please find below and/or attached an Office communication concerning this application or proceeding.

**Office Action Summary**

Application No.

09/506,717

Applicant(s)

HELSON, HAROLD E

Examiner

Ardin Marschel

Art Unit

1631

-- The MAILING DATE of this communication appears on the cover sheet with the correspondence address --

**Period for Reply**

A SHORTENED STATUTORY PERIOD FOR REPLY IS SET TO EXPIRE 3 MONTH(S) FROM THE MAILING DATE OF THIS COMMUNICATION.

- Extensions of time may be available under the provisions of 37 CFR 1.136(a). In no event, however, may a reply be timely filed after SIX (6) MONTHS from the mailing date of this communication.
- If the period for reply specified above is less than thirty (30) days, a reply within the statutory minimum of thirty (30) days will be considered timely.
- If NO period for reply is specified above, the maximum statutory period will apply and will expire SIX (6) MONTHS from the mailing date of this communication.
- Failure to reply within the set or extended period for reply will, by statute, cause the application to become ABANDONED (35 U.S.C. § 133).
- Any reply received by the Office later than three months after the mailing date of this communication, even if timely filed, may reduce any earned patent term adjustment. See 37 CFR 1.704(b).

**Status**

- 1) ☒ Responsive to communication(s) filed on 30 June 2003.
- 2a) ☐ This action is **FINAL**.                      2b) ☒ This action is non-final.
- 3) ☐ Since this application is in condition for allowance except for formal matters, prosecution as to the merits is closed in accordance with the practice under *Ex parte Quayle*, 1935 C.D. 11, 453 O.G. 213.

**Disposition of Claims**

- 4) ☒ Claim(s) 5-21 is/are pending in the application.
- 4a) Of the above claim(s) \_\_\_\_\_ is/are withdrawn from consideration.
- 5) ☐ Claim(s) \_\_\_\_\_ is/are allowed.
- 6) ☒ Claim(s) 5-21 is/are rejected.
- 7) ☐ Claim(s) \_\_\_\_\_ is/are objected to.
- 8) ☐ Claim(s) \_\_\_\_\_ are subject to restriction and/or election requirement.

**Application Papers**

- 9) ☐ The specification is objected to by the Examiner.
- 10) ☐ The drawing(s) filed on \_\_\_\_\_ is/are: a) ☐ accepted or b) ☐ objected to by the Examiner.
- Applicant may not request that any objection to the drawing(s) be held in abeyance. See 37 CFR 1.85(a).
- 11) ☐ The proposed drawing correction filed on \_\_\_\_\_ is: a) ☐ approved b) ☐ disapproved by the Examiner.
- If approved, corrected drawings are required in reply to this Office action.
- 12) ☐ The oath or declaration is objected to by the Examiner.

**Priority under 35 U.S.C. §§ 119 and 120**

- 13) ☐ Acknowledgment is made of a claim for foreign priority under 35 U.S.C. § 119(a)-(d) or (f).
- a) ☐ All b) ☐ Some \* c) ☐ None of:
1. ☐ Certified copies of the priority documents have been received.
  2. ☐ Certified copies of the priority documents have been received in Application No. \_\_\_\_\_.
  3. ☐ Copies of the certified copies of the priority documents have been received in this National Stage application from the International Bureau (PCT Rule 17.2(a)).
- \* See the attached detailed Office action for a list of the certified copies not received.
- 14) ☐ Acknowledgment is made of a claim for domestic priority under 35 U.S.C. § 119(e) (to a provisional application).
- a) ☐ The translation of the foreign language provisional application has been received.
- 15) ☐ Acknowledgment is made of a claim for domestic priority under 35 U.S.C. §§ 120 and/or 121.

**Attachment(s)**

- 1) ☒ Notice of References Cited (PTO-892)                      4) ☒ Interview Summary (PTO-413) Paper No(s). 14
- 2) ☐ Notice of Draftsperson's Patent Drawing Review (PTO-948)                      5) ☐ Notice of Informal Patent Application (PTO-152)
- 3) ☐ Information Disclosure Statement(s) (PTO-1449) Paper No(s) \_\_\_\_\_                      6) ☐ Other:

### **DETAILED ACTION**

The amendment, filed 6/30/03, has been approved for entry and has been entered and has overcome the previous rejections of record. Below are summarized new grounds of rejection which are applicable to the presently pending claims. Due to the setting forth of the new grounds of rejection, as summarized below, the finality of the Office action, mailed 4/23/03, is hereby withdrawn.

Applicants' arguments, filed 6/30/03, have been fully considered but they are not deemed to be persuasive. Rejections and/or objections not reiterated from previous office actions are hereby withdrawn. The following rejections and/or objections are newly applied. They constitute the complete set presently being applied to the instant application.

### **NEW MATTER**

Claims 11, 13, 14, and 16-18 are rejected under 35 U.S.C. 112, first paragraph, as failing to comply with the written description requirement. The claim(s) contains subject matter which was not described in the specification in such a way as to reasonably convey to one skilled in the relevant art that the inventor(s), at the time the application was filed, had possession of the claimed invention.

In claim 11, a limitation of queuing at least a subset of candidates by priority was added in a previous amendment. Consideration of the instant disclosure as filed, reveals that queuing has written basis in the specification as filed on page 8, line 17, through page 9, line 2, wherein priority queuing is limited to the ESVDs left over after the best of the possible ESVDs are actually pursued. This is a more limited disclosure

Art Unit: 1631

than that of the present claim 11 wherein any subset of candidates are queued by priority. The broader priority queuing in claim 11 therefore contains NEW MATTER. Priority queuing is also disclosed in the specification as filed on page 23, lines 1-10, wherein again only the inferior ESVDs are queued after the best ESVDs are separately analyzed. This again supports this NEW MATTER rejection of instant claim 11 which lacks any corresponding priority candidate queuing limitation, such as only for inferior ESVDs.

Claims 13 and 14 set forth the practice of a table which is configured to allow additional elements etc. to be added. This specific configuration of a table has not been found as filed and therefore is NEW MATTER. It is acknowledged that Table 1, for example, contains a list of elements etc., but that there is neither therein or elsewhere in the disclosure as filed a table which is specifically configured to allow additional elements etc. which supports this NEW MATTER rejection.

Claim 16 contains the limitation directed to "determining whether it is practical to produce a fixed bond representation of the chemical structure". This practicality determination has not been found as filed and is therefore NEW MATTER.

Consideration of the instant specification as filed reveals that on page 19, lines 7-10, a termination of steps of execution of the instantly claimed method may occur via an exhausting of possibilities or by exceeding an allocated amount of time. Neither of these cited termination reasons are generic regarding practicality as now determined in instant claim 16. It is acknowledged that termination via said exhausting or said exceeding an allocated amount of time may be specific practical limits to producing a

Art Unit: 1631

fixed bond representation, but that they are more limited than the broad and generic "determining whether it is practical" as in claim 16 which therefore supports the generic claim 16 practicality practice as containing NEW MATTER. Similarly, the "determining whether it is possible" limitation in instant claims 17 and 18 contain NEW MATTER for the same reasons as given above for claim 16.

### **NON-STATUTORY SUBJECT MATTER**

35 U.S.C. 101 reads as follows:

Whoever invents or discovers any new and useful process, machine, manufacture, or composition of matter, or any new and useful improvement thereof, may obtain a patent therefor, subject to the conditions and requirements of this title.

Claims 5-20 are rejected under 35 U.S.C. 101 because the claimed invention is directed to non-statutory subject matter.

Consideration of the "Computer-Related Inventions" section of the MPEP at section 2106, Part IV, subpart B, has revealed that the instant claims are directed to non-statutory subject matter without requiring performance of a result outside of a computer. Thus, the manipulation of data or conversion of data, in this case a method of system, which may be a software system, which manipulates chemical structure information and/or representation(s) is the claimed subject matter without any physical transformation outside of the computer. It is suggested that requiring some type of physical practice such as a display of information may overcome this rejection.

### **VAGUENESS AND INDEFINITENESS**

Claims 5-21 are rejected under 35 U.S.C. 112, second paragraph, as being indefinite for failing to particularly point out and distinctly claim the subject matter which applicant regards as the invention.

In claim 5, line 2, the practice of analyzing "a Kekule structure representation" is set forth. It is noted that consideration of the instant specification has failed to reveal a specific definition of the metes and bounds of what is meant by "a Kekule structure". The Background of the Invention section on page 1 of the specification describes a suggestion by Auguste Kekule that "double bonds were not fixed or localized, and depicted a benzene ring with a delocalized circle instead of alternating single and double bonds". In the first 3 lines of the "Summary of the Invention" section on page 1, the instant invention seems to be described as being directed to fixed bond information and, "In particular, a fixed bond representation...derived from a delocalized representation.". Consideration also of the instant Figure 1 reveals chemical structures with single and double bonds or, alternatively represented in a Kekule structure with a circle denoting delocalized double bonds. None of the above citations, nor any found elsewhere, as filed, however, limits Kekule structure practice to chemical structures with either one or more double bonds or circle representations of delocalized bonding. However, the extensive discussion in the disclosure as filed, including all of the chemical structures in the Figures, are directed to structures with at least some delocalized double bonds with corresponding fixed bond structures with at least one or more double bond(s) therein. This focus on double bond containing chemical structures as filed results in the metes and bounds of what is meant for the instant claim wording of the Kekule structures of the invention being vague and indefinite as to whether a double bond containing chemical is a limiting feature or not. One additional possible interpretation is that a lack of specific double bond limitations in the basic chemical

Art Unit: 1631

structure wording, either Kekule wording or fixed bond wording, of the instant claims makes the metes and bounds of the claims not commensurate in scope with the somewhat apparent double bond containing chemical disclosure in the specification. It is noted that the art includes a wide variety structures of chemical types in what is commonly referred to as Kekule structure representations. See, for example, Figures 1 – 3 of Morikawa [Computers Chem 20:159-165(1996)]; Figure 1 of Cash [J. Chem. Inf. Comput. Sci. 38:58-61(1998)]; and Table I of Graovac et al. [JACS 95:6267-6273 (1973)]. Clarification of the metes and bounds of the instant claim practice is requested via clearer claim wording as to what type(s) of chemicals are being analyzed etc. in the methodology of the instant claims.

### **PRIOR ART**

The following is a quotation of the appropriate paragraphs of 35 U.S.C. 102 that form the basis for the rejections under this section made in this Office action:

A person shall be entitled to a patent unless –

(b) the invention was patented or described in a printed publication in this or a foreign country or in public use or on sale in this country, more than one year prior to the date of application for patent in the United States.

Claims 5, 11, 15, and 20 are rejected under 35 U.S.C. 102(b) as being clearly anticipated by Graovac et al. [JACS 95(19):6267-6273 (1973)].

As noted above, the metes and bounds of what is meant by Kekule structure representation in the claims reasonably may be interpreted as being inclusive of a variety of such representations. In Graovac et al. the abstract summarizes the description therein as being directed to utilizing valence structures of hydrocarbon systems to produce a Kekule index which corresponds to Kekule-type valence

structures. These structures are evaluated via the empirical Fries rule to predict stability. Table I on page 6269 lists various Kekule structures which have been identified and evaluated via Kekule indices which are deemed to be practices as in lines 2-5 of instant claim 5. The indices are also deemed to be fixed bond information as required in the instant claims, such as in claim 5, line 8. Specific fixed bond structures are selected, as well as discussed, from said Table I on page 6269, right-hand column, lines 4-40, which anticipates selecting practice as in instant claim 5, lines 6-7. The ring system structures in said Table I are clearly polycyclic ring systems as required in instant claim 5, last 2 lines. These structures also depict the electronic state and valence distribution information via the bonding as required in instant claim 15. The reference also reasonably sets forth a system as in instant claim 20 as the reference is directed to a methodology system reasonably as in instant claim 20 which lacks any specific limitations which specify a system therein to exclude such a methodology system as in the reference. Several fixed bond structures in Table I and Tables II and III (page 6270) are lined up with the highest Kekule index as the left most structure with decreasing index to the right. See, for example, Table I, second row of structures directed to phenanthrene wherein the index goes from 0.913 (0.931) to 0.897 (0.890) which is a type of priority queuing as required in instant claim 11. Thus, these descriptions in Graovac et al. anticipate the above listed instant claims.

Claims 5, 7, 8, 10, 11, 15, and 19-21 are rejected under 35 U.S.C. 102(b) as being clearly anticipate by Morikawa [Computers Chem. 20:159-165 (1996)].



Similar to the above reference Morikawa discloses the analysis of Kekule structure representations of polycyclic chemicals with specific structures shown therein in Figures 1 – 3. These structures are specifically cited as being enumerated via programming language on page 160, left-hand column, lines 7-12, and in a computer calculation which starts on page 162, right-hand column, in a section entitled "COMPUTER CALCULATION AND DISCUSSION". These disclosures analyze, identify, evaluate K number with selection of specific structures thereof with also depicting production of fixed bond information as required in instant claims 5, 20, and 21. The bonding shown in the Figures also show the electronic state and valence distribution as in instant claim 15. Figure 2 shows queuing for priority via K number as also required instant claim 11. Portions of the structures in Figures 2 and 3 of the reference are non-cyclic or acyclic as required in instant claims 7 and 8. Figure 3 shows the pair of radicals as required in instant claim 10 which are lacked in one of the other Kekule structure representations which is left and up one row from the diradical representation. Certain structures as in Figures 1 - 3 of the reference include a monocyclic portion as required in instant claim 19.

No claim is allowed.

Papers related to this application may be submitted to Technical Center 1600 by facsimile transmission. Papers should be faxed to Technical Center 1600 via the Central PTO Fax Center. The faxing of such papers must conform with the notices published in the Official Gazette, 1096 OG 30 (November 15, 1988), 1156 OG 61 (November 16, 1993), and 1157 OG 94 (December 28, 1993)(See 37 CFR § 1.6(d)). The Central PTO Fax Center number is (703) 872-9306.

Any inquiry concerning this communication or earlier communications from the examiner should be directed to Ardin Marschel, Ph.D., whose telephone number is

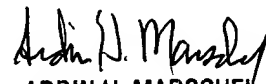
Art Unit: 1631

(703)308-3894. The examiner can normally be reached on Monday-Friday from 8 A.M. to 4 P.M.

If attempts to reach the examiner by telephone are unsuccessful, the examiner's supervisor, Michael Woodward, Ph.D., can be reached on (703)308-4028.

Any inquiry of a general nature or relating to the status of this application should be directed to Legal Instrument Examiner, Tina Plunkett, whose telephone number is (703)305-3524 or to the Technical Center receptionist whose telephone number is (703) 308-0196.

October 22, 2003

  
ARDIN H. MARSCHEL  
PRIMARY EXAMINER